LA-UR-80-2437

CONF-800857--1

TITLE: STATISTICAL MECHANICS OF SOLITONS

AUTHOR(S): ALAN BISHOP

SUBMITTED TO: "Physics in One-Dimension", Fribourg, Switzerland, August 25 - 29, 1980

DISCLAIMER

MASTER

University of California

LOS ALAMOS SCIENTIFIC LABORATORY
Post Office Box 1663 Los Alamos, New Mexico 87545
An Affirmative Action/Equal Opportunity Employer

UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

STATISTICAL MECHANICS OF SOLITONS

Alan Bishop
Theoretical Division, Los Alamos Scientific Laboratory
University of California
Los Alamos, New Mexico 87545

ABSTRACT

We broadly review the status of statistical mechanics theory (classical and quantum, statics and dynamics) for 1-D soliton or solitary-wave-bearing systems. Primary attention is given to (i) perspective for existing results with evaluation and representative literature guide; (ii) motivation and status report for remaining problems; (iii) discussion of connections with other 1-D topics represented in the Conference and elsewhere:

A) We introduce a general class of 1-D kink solitary-wave-bearing Hamiltonians[1] (x = scaled space, t = scaled time)

$$H = \int dx \{ \tfrac{1}{2}\phi_t^2 + \tfrac{1}{2}\phi_x^2 + V(\phi) \} \quad , \tag{1}$$

which includes for V the sine Gordon (SG), ϕ-four, double-SG, Eshelby, etc., potentials. Classical, low-T, static properties are now understood fully for the whole class (1), including striking universal T-dependencies. Complete agreement is obtained between transfer integral results and a "phenomenological" approach in terms of an effective gas of independent kinks and linear phonons -- if a (thermally) renormalized kink energy is used because of kink-phonon interactions. Static correlations are also described, emphasizing dependencies on the particular functions being correlated. Qualitative phenomenology at higher T is discussed since this is most relevant to topical applications (e.g. talks of J. R. Schrieffer, M. Steiner). Some modifications to the gradient coupling term in (1) are needed in, e.g., spin models. We discuss these and their effects.

B) Several "phenomenological" schemes for kink-phonon statistical mechanics have been used in the literature. They all amount to perturbation treatments about explicit kink profiles, accommodating "zero-frequency" modes by the introduction of "collective-coordinates."[2] These techniques are illustrated with a 1-D but 2-component order-parameter model, the ferromagnetic Heisenberg chain with easy-axis anisotropy.[3] We emphasize the equivalence of all collective coordinate schemes (including that in A) and discuss their limitations.

C) The status of dynamic correlation function calculations for class (1) will be summarized within both Hamiltonian and Fokker-Planck frameworks, emphasizing strongly nonlinear (soliton) signatures - see also talks of M. Büttiker and T. Schneider.

D) Kink-solitons and their statistical mechanics (certainly at low-T) are now very well understood and of little further interest. Much the most challenging problems remaining concern non-topological pulse or envelope solitons (of wide physical relevance). We illustrate these with the solitons, of the Toda lattice, a cubic Schrödinger equation, the continuum ferromagnetic Heisenberg chain, and the SG breather. A very appealing approach is to use the complete integrability of these strict soliton systems to transform to a natural action-angle variable (soliton) basis. Building on the introduction of D. W. McLaughlin, we investigate this approach to classical statistical mechanics and describe some generic problems for non-kink solitons.

E) Some of the problems in D) can be overcome if we consider quantum statistical mechanics. We summarize approaches and pertinent results for strict and non-strict soliton systems - more detailed discussion is given by K. Maki. In particular, we emphasize the quantization scheme for strict soliton systems due to Fadeev, et al., especially as applied to the X-Y-Z

Heisenberg chain. Connections with Bethe ansatz calculations for spin-½ XYZ chains (see also J. C. Bonner) and other exactly soluble quantum models (→ exactly integrable quantum models), allows some lessons to be drawn about soliton statistical mechanics.

F) Finally, we emphasize the ubiquity of the soliton concept in 1-D physics by noting its connections with so many 1-D problems (experimental and theoretical) discussed at this Conference and elsewhere.

1) J. F. Currie, J. A. Krumhansl, A. R. Bishop, S. E. Trullinger, Phys. Rev. B, in press (1980); R. M. De Leonardis and S. E. Trullinger, preprint (1980).

2) e.g. J. S. Langer, Adv. Phys. 14, 108 (1967).

3) A. R. Bishop, K. Nakamura, T. Sasada, preprint (1980).

4) e.g. E. K. Sklyanin, L. D. Faddeev, Sov. Phys. Dokl. 23, 902 (1978).

STATISTICAL MECHANICS OF SOLITONS

Alan Bishop
Theoretical Division, Los Alamos Scientific Laboratory
University of California
Los Alamos, New Mexico 87545

1. Introduction

I was asked to talk about the statistical mechanics (SM) of solitons (in 1-D). This is an almost open-ended brief -- indeed the "soliton" concept is one of the major unifying threads of low-D physics. Fortunately, at this Conference there are a number of inter-related soliton contributions. Here, I have decided to (i) indicate natural connections with other invited papers; (ii) survey what is known *rigorously* about soliton SM, what is conjectured, and what *important* open questions remain; (iii) emphasize SM of solitons rather than of soliton Hamiltonians. By this I mean that I will mostly stress what is known rigorously about "solitons" as (nonlinear) elementary modes. I contrast this with purely numerical results (e.g. from the transfer integral operator (TIO) or molecular dynamics (MD)) without interpretation or with *approximate* mode interpretations -- these are hopefully useful for experimental guidance and will be surveyed by SCHNEIDER. I will omit any discussion of *dynamics* here. Little is known rigorously; the many interesting questions concerning analytic, numerical or phenomenological approaches in Hamiltonian or Langevin frameworks will be surveyed by BUTTIKER and SCHNEIDER.

2. Representative Models

It would be inappropriate to restrict ourselves to solitons in the strict mathematical sense (see McLAUGHLIN): the soliton paradigm is far more pervasive [1,2]. Nevertheless, strict solitons systems are valuable test models and also of deep interest to the mathematical physicist. We include several below:

A. *Nonlinear Klein-Gordon (KG) class*: Sustained attention has been given [1-3] to this class of nonlinear Hamiltonians supporting kink-soliton excitations. The general Hamiltonian is defined on a dimensionless one-component field $\{\phi_n\}$ (lattice sites labelled by $\{n\}$) and has the form

$$\mathcal{H} = \sum A\ell\left\{\frac{1}{2}\dot{\phi}_n^2 + \frac{1}{2}c_0^2\ell^{-2}(\phi_{n+1}-\phi_n)^2 + \omega_0^2 V(\phi_n)\right\} . \qquad (1)$$

A sets the energy scale and ℓ is the lattice spacing. The continuum (or "displacive") limit ($c_0/\omega_0 \gg \ell$) is especially attractive theoretically:

$$\mathcal{H} = A\int dx\left\{\frac{1}{2}\dot{\phi}^2(x,t) + \frac{1}{2}c_0^2\,\phi_x^2(x,t) + \omega_0^2 V(\phi)\right\} . \qquad (2)$$

In either (1) or (2) the local potential $V(\phi)$ is the sole source of nonlinearity. Its only restriction is that it have at least two *degenerate* minima (at say $\phi = \phi_{1,2}$), with (for simplicity) local symmetry about the minima. This is sufficient to admit a topologically stable kink solution to the equation of motion from (2):

$$\ddot{\phi} - c_0^2\phi_{xx} + \omega_0^2\, dV/d\phi = 0. \tag{3}$$

The single-kink (or antikink) excitation translating with velocity v carries the field from $\phi_{1,2}$ to $\phi_{2,1}$ over a distance $\propto d(1 - v^2/c_0^2)^{1/2}$ ($d \equiv c_0/\omega_0$), and is found easily [1-3]. The single kink energy $E_K^{(v)}$ exhibits the same "relativistic" dependence (implicit in (3)): $E_K^{(v)} = E_K^{(0)}(1 - v^2/c_0^2)^{-1/2}$, $E_K^{(v)2} = E_K^{(0)2} + p^2c_0^2$; $E_K^{(0)} = M_K c_0^2$; $p = M_K v(1 - v^2/c_0^2)^{-1/2}$; $M_K = \sqrt{2}\, Ad\int_{\phi_1}^{\phi_2} d\phi\, |V(\phi)|^{1/2}$. Such kink solutions are in striking contrast to familiar small amplitude ($<<|\phi_1-\phi_2|$), approximate, harmonic ("linear phonon") solutions $\phi(x,t) - \phi_{1,2} \propto \exp[i(kx-\omega_k t)]$ with continuum (Debye) dispersion

$$\omega_k^2 = \omega_0^2 + c_0^2k^2 = \omega_0^2(1 + d^2k^2). \tag{4}$$

The nonlinear KG class contains several examples which have long been practice models for "soliton" SM. For example the "sine-Gordon" (SG) [$V(\phi) = 1 - \cos\phi$] is (effectively) considered in [4] and this and other periodic local potentials are studied in [5] (such as the Eshelby form $V(\phi) \propto (|\phi| - 1)^2$, periodically continued). Again the "ϕ-four" form [6] $V(\phi) = (\phi^2 - 1)^2/8$ is the most familiar of Landau expansions but many other such unbounded potentials are studied, as are potentials supporting several kink types, e.g. the "double SG" [7]. The important recent developments (§§3,4) are the *proof* of an exact kink statistical mechanics at low temperature (T), and of its validity for the *whole* class (2). (Differences between periodic and unbounded potentials *are* important at high-T or for dynamics.) The *discrete* lattice (c.f. (1)) also supports harmonic modes (with a trivially modified dispersion [1,2]) and kinks, but these interact increasingly strongly as d/ℓ decreases. Conveniently, however, many low v kink properties (e.g. energy, width) are only weakly affected unless $d \sim \ell$[8].

One other excitation must be mentioned. *Anharmonic* perturbation theory about $\phi_{1,2}$ suggests a tendency towards the formation of spatially and temporally coherent excitations: particle-like envelopes with an oscillatory internal motion. We refer to these generically as "breathers". (Indeed linear SG wave-trains are modulationally unstable to breather formation.) They are observed in MD simulations of ϕ-four or SG, and in deterministic simulations of several members of class (2) (corresponding to strong anharmonic effects as well as weak ones). Breathers are fundamentally different from kinks and lie at the heart of the interesting open areas in soliton SM. Breathers, ϕ_B, are only known (McLAUGHLIN) *analytically* in class (2) for SG, in which integrable (§5) case they in principle exhaust the "anharmonic phonon" spectrum:

$$\phi_B(x,t;\, v_B,\omega_B,x_0,\phi_0) = 4\tan^{-1}\psi_B, \text{ where } (\gamma = (1 - v_B^2/c_0^2)^{-1/2})$$

$$\psi_B = \frac{\left(\frac{\omega_0^2}{\omega_B^2} - 1\right)^{1/2} \sin\left[\gamma\omega_B\left(t - \frac{v_B}{c_0^2}(x - x_0)\right) + \phi_0\right]}{\cosh\left[\gamma d^{-1}(x - x_0 - v_B t)(1 - \omega_B^2/\omega_0^2)^{1/2}\right]} \tag{5}$$

B. *Multi-component generalizations*: A number of generalizations of class A to multi-component fields have been studied. These are immediately relevant for problems with multi-component order parameters, leading to *coupled* nonlinear equations. Kink and other soliton solutions are known (sometimes analytically) for many of these but little has been accomplished in incorporating them in a SM theory at the level we will report for class A. Two exceptions should be noted. First, the Heisenberg ferromagnet with Ising anisotropy, see C. Second, a natural generalization of class A to a complex order parameter with *2-fold* symmetry breaking (see [9,10]) exhibits both ϕ-four and SG-like kinks and a mean field *bifurcation*. SM of this model has revealed a possible role for an additional non-topological excitation indicated in numerical simulations [10].

C. *The Heisenberg ferromagnet and relations*: Spin Hamiltonians (classical and quantum) have gained renewed attention from soliton devotees in recent years for several reasons. Models of easy-plane ferro- or anti-ferromagnets with easy-plane magnetic fields (STEINER) have mostly been limited to SG approximations (possibly with periodic coupling, c.f. (1) ([11,12]; §3.2). More generally we will refer here to the classical Heisenberg-Ising-XY Hamiltonian

$$\mathcal{H} = -J\sum_n \vec{S}_n \cdot \vec{S}_{n+1} - A\sum_n S_n^z S_{n+1}^z, \tag{6}$$

where $\{\vec{S}_n\}$ are classical spin-vectors $\vec{S}_n = S(\sin\theta_n \cos\phi_n, \sin\theta_n \sin\phi_n, \cos\theta_n)$ ($|\vec{S}_n| = S$). The Landau equations of motion are $d\vec{S}_n/dt = \{\mathcal{H}, \vec{S}_n\}$. The exchange anisotropy in (6) might be replaced or supplemented with local anisotropy, e.g. $A\sum_n (S_n^z)^2$. Major interest centers on the complete integrability of (6) in the *continuum* limit [12] and of the corresponding spin-½ quantum chain (c.f. 5). Here we simply give the flavor of soliton types by recording a few single-soliton forms we need. The continuum ferromagnet with uniaxial local anisotropy [Hamiltonian density $\mathcal{H}(x) = -J(1 - \frac{1}{2}(d\vec{S}/dx)^2) - A(S^z)^2$] has *static* π-domain wall solutions [13,11] (distances in lattice spacings)

$$S^z = S\tanh\left(\frac{x-x_0}{d}\right); \quad S^\pm = S e^{\pm i\phi_0}\,\mathrm{sech}\left(\frac{x-x_0}{d}\right)$$
$$S^\pm = S^x \pm iS^y; \; d = (J/2A)^{1/2} \tag{7}$$

These should be contrasted with familiar spin waves having continuum dispersion (c.f. (4))

$$\omega_k = 2A + Jk^2. \tag{8}$$

Notice that there are no simple *dynamic* generalizations of these walls (unlike (2A)). In fact the natural dynamic modes are *envelope* solitons in which (θ,ϕ) are intrinsically coupled. (The same is true for exchange easy-axis anisotropy.) General expressions are rather cumbersome [12,13] and will not be given, but the pulse amplitude → π (~ bound wall-antiwall) as its translation velocity → 0. In the isotropic Heisenberg limit, the pulse (velocity v) is

$$\cos\theta(x,t) = 1 - 2b^2\mathrm{sech}^2[b\tilde{\Omega}\ \ (x - x_0 - vt)]$$
$$\phi(x,t) = \phi_0 + \Omega t + (v/2JS)(x - x_0 - vt) \qquad (9)$$

with $b^2 = 1 - v^2/(4JS\Omega)$; $\Omega = JS\tilde{\Omega}$. The pulse has energy $E = 16JS^3|M^z|^{-1}\sin^2(P/4S)$, with linear momentum $P = 4S\sin^{-1}b$ and z-component of angular momentum $M^z = -4bS\Omega^{-1}$. Importantly, there is a gauge equivalence [15] between the above continuum spin equations and the continuum nonlinear (cubic) Schrödinger equation (see McLAUGHLIN). Both systems are completely integrable (§5) and the envelope soliton solutions to cubic Schrödinger require four action and angle variables ($\sim x_0$, v, ϕ_0, Ω in (9)) for specification as for SG breathers (5). Amongst integrable Hamiltonians we also mention the Toda lattice (see McLAUGHLIN). Although a contrived lattice dynamics, it supports the third typical soliton variety, *pulses*. In addition it is certainly the most studied *discrete* integrable Hamiltonian (c.f. §5).

3. Exact Analytic Results: Transfer Integral Operator (TIO)

3.1 Statics: Nonlinear KG Class

The TIO, especially as applied to 1-D Hamiltonians with nearest neighbor couplings (e.g. §2), has a dense history [1,2,6,11,16] with extensive data (both published and unpublished). Recent attention to soliton phenomenology (§4) has generally encouraged more analytic investigation, particularly at low T. We have described the TIO for nonlinear KG Hamiltonians in detail elsewhere [1,2]. A few central results will suffice here. We consider the discretized form (1) and write the *classical* partition function $Z = Z_\pi Z_\phi$

$$Z_\pi = (2\pi A\ell/\beta h^2)^{N/2} \qquad (10)$$

$$Z_\phi = \sum_n \exp(-\beta A\omega_0^2 L\epsilon_n) \qquad (11)$$

Here $L = N\ell$ (N = number of lattice sites), h is Planck's constant. The quantities $\{\epsilon_n\}$ in the "configurational" (i.e. potential-energy) partition function expression (11) are the eigenvalues of the TIO [1,2]. The TIO eigenfunctions ($\{\psi_n(\phi)\}$) constitute a complete orthonormal set on $(-\infty, +\infty)$. In the thermodynamic limit only the lowest eigenvalue ϵ_0 is important to Z_ϕ or, for instance [2,16], the (potential) free energy density $F_\phi \equiv -L^{-1}\beta^{-1}\ln Z_\phi$:

$$F_\phi \xrightarrow{L\to\infty} A\omega_0^2\epsilon_0. \qquad (12)$$

Equilibrium correlation functions, however, depend on both TIO eigenvalues *and* functions [2,16]: $C_g(x) \equiv \langle g(\phi(x))g^*(\phi(0))\rangle \xrightarrow{L\to\infty} \sum_n |\langle n|g(\phi)|0\rangle|^2 \exp(-x/\lambda_n)$. Here g is an arbitrary function of ϕ and the "n-th correlation length" $\lambda_n = [\beta A\omega_0^2(\epsilon_n - \epsilon_0)]^{-1}$. In some ("kink-sensitive") cases only the first excited level with non-zero matrix element is important [1,2,17]. In writing (11) and therefore (12), etc., we have assumed *periodic* boundary conditions $\phi_{N+1} = \phi_1$. These are readily varied within the TIO formalism [2,18] and this is sometimes physically necessary (e.g. for discommensuration arrays - see BAK); e.g. rigid or free boundaries with a fixed or floating "winding number" ($\equiv(\phi_N-\phi_1)/2\pi$ in SG). These considerations will usually not affect *intensive* quantities such as F_ϕ. Such boundary conditions will of course influence the kink-antikink density (§4).

If we wish to interpret the formally exact TIO results in terms of "elementary" nonlinear modes (§2A), the displacive limit $d \ll \ell$ affords most analytic control. To $O(\ell/d)$ the TIO can [2,16] be replaced by a Schrödinger-like ($\hbar \to T$) *differential* eigenvalue equation for $\Psi(\phi) \equiv \exp[-\frac{1}{2}\beta\ell A\omega_0^2 V(\phi)]\Phi(\phi)$:

$$\hat{H}(\phi)\Psi_n(\phi) = \epsilon_n\Psi_n(\phi)$$
$$\hat{H}(\phi) = -(2m^*)^{-1}d^2/d\phi^2 + V(\phi) + V_0 \,, \tag{13}$$

with $m^* = A^2\omega_0^2c_0^2\beta^2 \propto \left(\beta E_K^{(0)}\right)^2$ and $V_0 = (2\beta\omega_0^2\ell A)^{-1}\ln(Ac_0^2\beta/2\pi\ell)$. In terms of experimental applicability we note [8] that effects on eigenvalues from using (13) instead of the true TIO are at most a few percent unless $d \lesssim 2\ell$. The two lowest eigenvalues deduced from (13) are shown as a function of T in fig. (3) of [19]. Note that for periodic potentials $V(\phi)$ as in SG we have a band structure problem ((13) is the Mathieu equation for SG), with eigenvalues $\epsilon_{n,k}$ labeled by a "band" index $n(= 0,1,2,---)$ and "wave-vector" k in the first Brillouin zone ($-\frac{1}{2} < k \leq \frac{1}{2}$). The corresponding eigenfunctions have Bloch form [2]. Fig. (3) of [19] shows the lowest two characteristic eigenvalues (top and bottom of the first band); these correspond most closely to the lowest two levels of ϕ-four-like models. ϵ_0 and ϵ_1 converge rapidly for $k_BT \lesssim 0.2\, E_K^{(0)}$ (i.e. $m^* \gg 1$). Indeed, in this regime, they can be usefully analyzed [2,6] as tunnel-split single-well oscillator levels: $\epsilon_0 = E_0 - t_0$; $E_0 = \frac{1}{2}m^{*-1/2} + O\left(\beta E_K^{(0)}\right)^{-1}$. The tunneling term can be extracted by standard WKB schemes, and for class 2A is found to have a "universal" form giving [2]

$$F_t \equiv -A\omega_0^2 t_0 = -\eta A\omega_0^2\pi^{-1/2}\left(\beta E_K^{(0)}\right)^{-1/2}\exp\left(-\beta E_K^{(0)}\right). \tag{14}$$

η is a numerical coefficient depending on the particular $V(\phi)$: e.g. $\eta(SG) = 16\sqrt{2}$; $\eta(\phi^4) = 2\sqrt{2/3}$. Eq. (14) includes a correction factor to WKB ($(\pi/e)^{1/2}$) common to class 2A (at asymptotic low T) [20]. It should seem physically plausible that E_0 is related to harmonic (and anharmonic) phonon modes, and t_0 to kink configurations. This suggestion [6] is now verified for all class 2A (§4).

We will not dwell here on numerical solutions of (13) (or the TIO) for non-asymptotic (high or low) T regimes. These are straightforward and have been abundant since at least [16] for class 2A and many of the spin Hamiltonians 2C: Renewed interest has been stimulated by speculations on certain magnetic chains (see STEINER). In this context information from the TIO on *correlation* functions (see below (12)) is important. In particular, certain interesting correlations in planar (classical) *anti*-ferromagnets are dominated by kink-*sensitive* functions for which a simple Ising-like kink phenomenology can be constructed. (Solitons enter through eigen*value* tunnel-splitting.) By contrast, corresponding properties in corresponding *ferro*magnets are determined from kink-*insensitive* functions, which are dominated by anharmonicity, with kinks only entering weakly through a careful eigenfunction study. Phenomenology is then more difficult. We do not have space to develop these interesting topics here [1,17].

3.2 Statics: Other Models

Many of the models in 2A-C have been studied via the TIO. Tunnel-splitting ($\rightarrow$ *kink* solitons) are not found in the Toda lattice [21,22]. *Periodic* nearest-neighbor coupling in §2A is possibly interesting in view of planar approximations to easy-plane magnetic chains. This is considered in detail in [11]. The SG approximation [$\cos(\phi_{n+1}-\phi_n) \to 1 - \frac{1}{2}(\phi_{n+1}-\phi_n)^2$] is generally found to be reasonable (for static properties) in the displacive regime at low T, with one essential provision. This is that the TIO or (13) are restricted to the range $(-\pi,\pi)$ not $(-\infty, +\infty)$. Thus, even in a SG approximation, we must only use 2π-periodic Mathieu functions, not the whole band structure. This has obvious consequences, particularly for correlation functions since certain previously finite matrix elements in the TIO expression for $C_g(x)$ (below (12)) may be excluded [11].

TIO applications to coupled scalar field Hamiltonians are also numerous (e.g. [9,10]). In some cases analytic attention to tunnel-splitting features can be profitable: see for instance [10] for a complex order parameter model (2B). Spin Hamiltonians (2C) are also extensively documented (see [14]): We report one example here for later use; the continuum uniaxial Heisenberg ferromagnetic (c.f. (6) - (9))[14]: Using the TIO formalism, the free energy density is [14]

$$F = \beta^{-1}\ln(\beta J/2\pi) - J + \epsilon_0 , \tag{15}$$

where ϵ_0 is the lowest eigenvalue of a (two-variable) "hindered rotator" transfer matrix eigenvalue equation, which can be transformed into the single-variable form

$$\begin{aligned} &d^2\psi(u)/du^2 + V(u;E)\psi(u) = 0 \\ &V(u;E) = -\tfrac{1}{4}(\beta E_W)^2[(E/A) + \tanh^2 u]\,\mathrm{sech}^2 u. \end{aligned} \tag{16}$$

The eigenvalue problem (16) differs from the Schrödinger form (13), but for $|E| < A$ (sufficient for ϵ_0) a very similar *tunneling* problem emerges. With the same low-T WKB approach, we find [14] $\epsilon_0 = E_0 - t_0$ with $E_0 = -A[1-4(\beta E_W)^{-1} + O(\beta E_W)^{-2}]$ and

$$t_0 \xrightarrow{T\to 0} 4(e/\pi)d^{-1}\beta(\beta E_W)\exp(-\beta E_W). \tag{17}$$

The factor (e/π) is cancelled by the same WKB corrections which removed the factor $(e/\pi)^{\frac{1}{2}}$ for class 2A. The important difference from the *one*-component class 2A is the prefactor βE_W in (17): for class 2A this appears universally as $(\beta E_K^{(0)})^{\frac{1}{2}}$ (c.f. (14)). This universal feature of class 2A can be understood (§4) very physically in terms of the phase-shifting effect of kinks on the extended harmonic excitations and the related zero-frequency kink translation mode. The spin model signature βE_W can be understood equally physically (§4), by recognizing *two* degrees of freedom for fluctuations, and *two* symmetries - spin-rotation about the easy-axis as well as translation, (7).

4. Nonlinear Mode Phenomenology

4.1 Low-T Statics: Non-interacting Kinks

Several *equivalent* schemes have been described in the last 20 years (e.g. [5,23,24] which evaluate various statistical properties of models exhibiting *kink*-solitons by explicitly recognizing those nonlinear configurations "or collective co-ordinates". Basically, these schemes are all attempts to build a "phenomenological" representation of a partition function around non-perturbative steepest descent or saddle-point trajectories. Examples from class 2A have been popular, but most schemes are more general (below). Typically, an exact phenomenology is possible at low k_BT (<< kink energy) because kink-kink interactions can be neglected and we only need to analyze the effect of a *single* kink on the *harmonic* modes. One then finds that "zero-frequency" modes, neglecting continuous symmetries, play a central role. We begin by summarizing the approach of CURRIE, et al. [2] since this has been applied in generality to class 2A, and leads to some more sophisticated ideas in §5. Complete details can be found in [2]. Extended harmonic wave forms ("phonons") are modified in the neighborhood (scale d) of a kink and most importantly their *density of states is changed*. This nonlinear feature is also central to perturbation theories and to the treatment of quantum or critical fluctuations about nonlinear configurations. We can handle the problem relatively easily because of the assumption of a simple isolated kink. Analyzing *linear* oscillations about a kink is well-known from stability theory [2,24]. The spectrum of small oscillations, $\chi(x,t) = f(x)e^{-i\omega t}$, comprises both bound (i.e. spatially-localized) and continuum (i.e. extended) states. Since the general continuum Hamiltonian (2) is *translationally* invariant there must be a "zero-frequency" (ω=0)("translation" or Goldstone) mode describing rigid kink translations. In linear order this corresponds to the lowest member of the bound state spectrum: $\omega_{b,1}^2 = 0$, $f_{b,1}(x) \propto d\phi_K^{(0)}(x)/dx$. In addition there may, depending on the potential $V(\phi)$, be $(N_b - 1)$ finite frequency bound states $(0 < \omega_{b,n} < \omega_0;\ n = 2, \ldots, N_b)$ describing harmonic kink-shape oscillations. E.g. for SG or double quadratic (§2A) $N_b = 1$; for ϕ-four $N_b = 2$. The remaining continuum spectrum (with wave-vector k) has dispersion $\omega_k^2 = \omega_0^2 + c_0^2k^2$, unchanged by the kink presence (eq. (4)). Only the asymptotic behavior of $f_k(x)$ is important below: the most general form is [2] $f_k(x) \xrightarrow{x\to\pm\infty} A_k \exp[i(kx\pm\frac{1}{2}\Delta(k))] + B_k \exp[-i(kx\pm\frac{1}{2}\Delta(k))]$. Here $\Delta(k)$ is a *phase-shift* (depending on $V(\phi)$). In fact SG and ϕ-four belong to a class [2] with *reflectionless* scattering (B_k=0). This is of *no* physical consequence in the present context but implies some mathematical simplicity which has made these examples popular demonstrations. The parallels with other scattering problems should already be evident and it will not be surprising that only *asymptotic* scattering data is important (i.e. the phase-shift). This contains information about the bound states and also about *conservation* of states. These are not well-posed questions in a continuum; we also want to make contact with the discrete TIO results (§3), so we consider a large system $L(N = L/\ell)$ and impose (e.g.) periodic boundary conditions on $\{f_k(x)\}$. [We will use the *continuum* $f_k(x)$, $\Delta(k)$, which is strictly inconsistent, but has been validated for our purposes to leading order in ℓ/d [25]. It *is* essential to use the discrete phonon dispersion.] We see that the phonon density of states is changed by the presence of a kink: $\rho(k) = \rho_0 + \Delta\rho(k)$; $\rho_0 = L/2\pi$, $\Delta\rho(k) = (2\pi)^{-1}d\Delta(k)/dk$. Conservation of states is assured by a form of Friedel sum rule: $P\int dk\Delta\rho(k) = -\pi^{-1}\Delta(0+) = -N_b$. $P \equiv$ principal value.) We can view this as "trapping" of phonon states by the kink - a precise mechanism for *sharing degrees of freedom in a nonlinear system*.

Procedural steps to a kink gas phenomenology are now straightforward. We will *assume* that kinks (and antikinks) form an ideal gas (at low T), but we *cannot* assume an independent phonon spectrum: the available phonon phase space is unavoidably dependent on the kink presence (and velocity, via a "Lorentz boost" - below). This *precludes* partition function factorization as truly independent excitations. The phonon free energy density associated with ρ_0 is $F_0 = (k_BT/2\pi)\int_{-\pi/\ell}^{\pi/\ell} dk\,\ell n(\beta\hbar\omega_k)$, i.e.

$$F_0 \xrightarrow{d>>\ell} k_BT[\ell^{-1}\ell n(\hbar\omega_0\beta d/\ell) + (2d)^{-1}], \qquad (18)$$

which is *precisely* identified with harmonic oscillator pieces in the TIO formalism ($O(k_BT/E_K^{(0)})$: $F_o \equiv A\omega_0^2E_0 - k_BTL^{-1}\ln Z_\Phi + A\omega_0^2V_0$ (see (10), ( )). Assuming independent kinks (i.e. additive phase shifts), the *change* in phonon free free energy density from $\Delta\rho$ is (for N_K kinks with velocities $\{v_i\}$ and $N_{\bar K}$ antikink with velocities $\{\bar v_i\}$) $\Delta F(\{v_i,\bar v_i\}) = \Sigma_i\Delta F(v_i) + \Sigma_i\Delta F(\bar v_i)$, with the single kink contribution

$$L\Delta F(v) = k_BT P\int_{-\pi/\ell}^{\pi/\ell} dk\Delta\rho(k;v)\ln(\beta\hbar\omega_k)$$

$$+ k_BT\sum_{n=2}^{N_b}\ln(\beta\gamma\hbar\omega_{b,n})$$

$$\xrightarrow{\ell<<d} k_BT\sum_{n=2}^{N_B}\ln(\beta\gamma\hbar\omega_{b,n}) - k_BTN_b\ln(\beta\hbar\omega_o)$$

$$+\frac{k_BT}{2\pi}P\int_{-\infty}^{\infty}dk\,\frac{d\Delta(k;v)}{dk}\ln(1 + k^2d^2)^{\frac{1}{2}}. \qquad (19)$$

We have kept track of "relativistic" dependencies (γ) in (19) - N.B. $\Delta(k;v) = \Delta(\gamma[k-v\omega_0c_0^{-2}(1 + k^2d^2)^{-\frac{1}{2}}];0)$. In both (18) and (19) we have used a high T limit ($k_BT >> \hbar\omega_0$ but $<< E_K^{(0)}$) of the quantum harmonic oscillator free energy expression to be consistent with the *classical* TIO. For use in §5, consider (19) for the SG case. Using the well-known phase shift formula (below), a simple contour integration yields $L\Delta F(v) = -k_BT\ln[\beta\hbar\omega_o(1 + \gamma)]$. As in quantization schemes [3], it is convenient to associate $\Delta F(v)$ with the *kink* (as a kink "self-energy"). A grand canonical partition function G can then be constructed for *ideal gases* of kinks and anti-kinks but with *renormalized energies*:

$$E_K^*(\gamma) \equiv \gamma E_K^{(0)} + L\Delta F(\gamma) \qquad (20)$$

We have effectively already integrated over phonon degrees of freedom. Thus, with the independent kink assumption, $G(T,L,\mu_K,\mu_{\bar K}) = \exp(-\beta F_0)G_KG_{\bar K}$ with

$$G_K(T,L,\mu_K) = \sum_{N_K=0}^{\infty} e^{\beta\mu_KN_K}\,Z_K(N_K), \text{ etc.}$$

$$Z_K(N_K) = (N_K!)^{-1}\left[h^{-1}\int_0^L dq_K\int_{-\infty}^{\infty}dp_K e^{-\beta E_K^*(p_K)}\right]^{N_K}. \qquad (21)$$

q_K is a kink position co-ordinate, p_K its momentum (§2A), and μ_K the chemical potential. For periodic boundary conditions we set $\mu_K = \mu_{\bar K} = 0$ after any thermodynamic manipulations. Standard thermodynamic formula lead [2] to explicit expressions for, e.g., free energy, specific heat, internal energy, kink density [$n_K^T = n_K + n_{\bar K} = 2(\beta L)^{-1}(\partial\ln G_K/d\mu_K)(\mu_K = 0)$]. Indeed the momentum integral in (21) can be performed exactly giving (see also [26])

$$n_K^T(T) = 2(\pi d)^{-1}\left\{\beta E_K^{(0)}[K_0(\beta E_K^{(0)}) + K_1(\beta E_K^{(0)})] + K_1(\beta E_K^{(0)})\right\} \tag{22}$$

$$\xrightarrow{\beta E_K^{(0)} \gg 1} \; 2(2/\pi)^{\frac{1}{2}} d^{-1} (\beta E_K^{(0)})^{\frac{1}{2}} \left[1 + \frac{5}{8} (\beta E_K^{(0)})^{-1} + O(\beta E_K^{(0)})^{-2}\right] e^{-\beta E_K^{(0)}} . \tag{23}$$

(K_0, K_1 modified Bessel functions) and $F = F_0 - k_B T n_K^T$. This last result agrees *exactly* with the TIO result (see (14)) to $O(\beta E_K^{(0)})^0$ in the parentheses of (23).

We could have achieved this low-T result *universally* for class 2A by working with the $\Lambda(k;0)$ only and expanding the momentum integral to Gaussian order (i.e. $\gamma E_K = E_K^{(0)} + \frac{1}{2}M_K v^2$). The universal T-dependence found by TIO (§3.1) then follows easily [1]. Indeed a general *low-T* n_K formula can be obtained [7] which does not require *explicit* knowledge of the kink waveform or small oscillations about it (i.e. asymptotic phase-shifts and kink vibration modes: there is a general cancellation [7]) - these are only needed implicitly via an integral involving $V(\phi)$ and the location of its degenerate minima. This result can also be derived within other collective mode formalisms (c.f. §4.2). Of course information on the perturbed "phonons" requires case-by-case small oscillation study. Having appreciated the significance of E_K^*, it is a simple textbook ideal gas calculation to introduce kink chemical potentials and handle phenomenology for varying boundary conditions, multi-kink species (§2A), and topological restrictions (e.g. kink-antikink ordering in ϕ-four). Agreement with TIO results has been obtained [26].

4.2 Equivalent Low-T Approaches

Our conclusion from §3.1 is that static phenomenology for class 2A [illegible] is complete and of little further interest. However, it is important to emphasize the equivalence of all competing "collective-co-ordinate" phenomenologies [5,23,24]. An example is probably best. Class 2A examples can be found in several references [5,24], so we present instead a more recent example [14] with *two* zero-frequency modes: the Ising symmetry ferromagnetic (§§2C,3.2). Of the several formalisms available we choose a collective co-ordinate scheme for evaluating the partition function in a steepest descent approximation, which emphasizes the very close connections between treatments of "inhomogeneous" states in different problems [14] - metastable state decay, disordered systems, quantum tunneling, nuclear physics, nucleation theory (see BÜTTIKER), quantization schemes (see MAKI). The method discussed at length by Langer [23] evaluates the classical partition function in a path integral representation by a steepest descent calculation with Gaussian corrections. To this end a normal mode ("linear stability") analysis must be performed about (nonlinear) solutions to the governing equations of motion, as in §4.1. The original functional integration can then be replaced by integrations over the normal mode amplitudes. However, continuous symmetries have to be treated specially, since large fluctuations must be accommodated properly - e.g. rigid translations (x_0 in (7)). We therefore exclude zero-frequency eigenmodes from the normal mode set and integrate separately over the corresponding collective co-ordinate (e.g. x_0), introducing appropriate Jacobians of transformation and ensuring orthoquality w.r.t. zero eigenfunctions. Modifications to the fluctuation (e.g. spin-wave) spectrum due to nonlinear excitations are explicit via effects on the density of states, as in §4.1. Here we will make use of a slight generalization of the technique to O(n) symmetry spin models [14], with the further modification that our single-site anisotropy model has only O(2) symmetry. Thus *two* continuous symmetries (rotation (ϕ_0) and translation (x_0)) must be treated specially.

First consider the single-wall sector partition function, Z_1. Following [23] we find ($S \equiv 1$)

$$Z_1 = \exp(N\beta(A+J) - \beta E_W) \int [d\eta][d\eta^*][dS_\xi] \exp(-\beta \int \eta^* M \eta \, dx) \qquad (24a)$$

$$= \exp(N\beta(A+J) - \beta E_W)(\det \mathcal{J})((2\pi)^N/\det(\beta M)) \qquad (24b)$$

with $\det \mathcal{J} \equiv \det \mathcal{J}_{\phi_0} \cdot \det \mathcal{J}_{x_0}$ (below). To derive (24) we have used the Ising symmetry and transformed to a local co-ordinate frame rotating with the wall (W) profile (7): $S^x = S_\xi \cos\theta_W + S_\zeta \sin\theta_W$, $S^y = S_\eta$, $S^z = -S_\xi \sin\theta_W + S_\zeta \cos\theta_W$. To Gaussian fluctuation order we find $\int dx \mathcal{H}[\vec{S}(x)] \cong -(A+J)N + E_W + \int \eta^* M \eta \, dx$, where $\sqrt{2}\, S_\zeta = (\eta + \eta^*)$, $\sqrt{2}\, S_\eta = -i(\eta - \eta^*)(\ldots \ll 1)$ and the stability operator $M = -Jd^2/dx^2 + 2A \cos 2\theta_W(x)$. This stability operator is familiar from the stability analysis for SG kinks [2](c.f. §4.1). The eigenspectrum comprises a "zero-frequency" bound state, f_0, describing rigid translations (x_0), and a continuum of "scattering states", f_k: $M(x)f(x) = Ef(x)$; $E_0 = 0$, $f_0 = (2d)^{-1/2}\mathrm{sech}(x/d)$; $E_k = 2A(1+k^2d^2)$, $f_k = (2\pi)^{-1/2}(1+k^2d^2)^{-1/2}\exp(ikx) \cdot [kd + i \tanh(x/d)]$. As in §3.1, the density of scattering states is $\rho(k) = \rho_0(k) + (2\pi)^{-1} d\delta(k)/dk$, where $\rho_0 = L/2\pi$ and the phase-shift $\delta(k) = \pi k/|k| - 2\tan^{-1}(kd)$. The last term in (24b), representing the scattering state contributions, can then be evaluated after straightforward integrations (c.f.[23]): $(2\pi)^N/\det(\beta M) = \exp[-\int dE\, \rho(E) \ln(\beta E/2\pi)] = [4A\ldots/\ldots] \cdot [\exp(-N \ln(\beta J/2\pi) + N(2A/J)^{1/2}]$. The second term is the contribution from free spin waves (ρ_0) (using a discrete dispersion and taking the limit $d \to \ldots$ as in §4.1) and the first term describes the effect of the *change* in the density of states $\Delta\rho$. The second term in (24b) describes contributions from the wall symmetry modes. As in [23], $\det \mathcal{J}_{x_0} = \int dx_0 \ldots dx \ldots \vec{S}_W/\partial x_0 \ldots = N(2/d)^{1/2}$. The co-ordinate transformations above were designed to suppress the rotational symmetry about the easy-axis. However, the full stability *matrix* for the wall contains a second zero-frequency mode $\propto \vec{S}_W^{\perp}$ (from $\partial\vec{S}_W/\partial\phi_0$) ($\vec{S}^{\perp} \equiv (S^x, S^y)$), reflecting the rotational symmetry in spin space [14]: $\det \mathcal{J}_{\phi_0} = \int d\phi_0 \ldots \vec{S}_W \ldots dx \ldots = 2\pi \int dx\, \mathrm{sech}^2(x/d) \ldots = 2\pi(2d)^{1/2}$. Gathering results, we have (suppressing the trivial ground state energy $-N(A+J)$) $Z_1 = \exp[-N(2A/J)^{1/2} - N\ln(\beta J/2\pi) - \beta E_W] \cdot (4\pi N) \cdot (4A\ldots/\ldots)$. At low T ($\ll E_W/k_B$) (i.e. low wall density), this single wall sector calculation can be extended to the multi-wall regime [14]. The total partition function Z_T is obtained from a partial exponentiation of Z_1, with associated free energy per spin $\tilde{F} = -\beta^{-1}N^{-1}\ln Z_T$:

$$\tilde{F} = 4Ak_BT/L_W + k_BT\ln(\beta J/2\pi) - 16A\exp(-\beta E_W). \qquad (25)$$

Eq. (25) must be compared with the transfer integral result (15), (17):

$$F = 4Ak_BT/L_W + k_BT\ln(\beta J/2\pi) - 16(e/\pi)A\exp(-\beta E_W). \qquad (26)$$

We see that F and $\tilde{F}$ agree exactly except for the purely numerical factor (e/π), which can be removed by improved evaluation of tunneling integrals, as remarked in §3.2. Most importantly, we see that the dominant low-T dependence is precisely reproduced *if* we account for all zero-frequency modes and associated scattering state phase-shifts.

4.3 Higher-T

Since we wish to emphasize rigorous mode phenomenology, it is important to stress how *little* is known beyond asymptotic low-T (except at trivial high T, where a soliton basis is a poor starting point), both for statics and even more for dynamics. TIO numerics are only consistency checks for plausible phenomenologies [17]. MD simulations (SCHNEIDER) provide very visual information on collision channels for strongly nonlinear modes and motivate approximate phenomenologies. In many cases there is little doubt about the fundamental role of kinks or other nonlinear modes but treatment of mode interactions is ad-hoc or perturbational. Of course such phenomenologies can be valuable theoretical and experimental guides if they are not used beyond their regimes of validity. For example, estimates [19] of kink-antikink density from appropriate correlation lengths within TIO show how n_K is decreased w.r.t. the low-T expression (23). Very little is known about virial kink-kink interactions. Expansion of the in-well oscillation contribution E_0 (see §3.1) in powers of $k_BT/E(0)$ can be identified exactly term-by-term as an anharmonic "phonon" expansion [2]. However, this does not recognize the intrinsic spatial and temporal coherence of modes such as "breathers", even though these are very apparent in SG-like and ϕ-four-like model simulations, and can be described in anharmonic expansions. The same problem arises if perturbation expansions are made (as in collective-co-ordinate schemes) about an N-kink configuration [24]. A related problem occurs in all collective co-ordinate schemes [24] where kinetic and configurational partition function components are separated (as in TIO). It is then difficult to assign parts of Z, to individual nonlinear modes. For low-T kinks this is possible; for breathers and similar pulse or envelope solitons it is a problem. In principle, *exactly* integrable Hamiltonian systems provide a means of overcoming this difficulty and extending rigorous phenomenology to arbitrary T. In practice difficulties remain, but we consider such systems a major soliton SM cutting edge!

5. Integrable Hamiltonian Systems

The beautiful mathematics developed in the last 10 years for integrable Hamiltonians has been introduced by McLAUGHLIN. For SM the major interest is that canonical transformations are prescribed to (generalized) "action-angle" variables or natural "nonlinear normal modes" - e.g. in the sense that they form a complete orthogonal set. (The Hamiltonian separability is a generalization of that found in *linear* perturbation order for a kink, §4.1.) Nonlinear modes necessarily interact, but in these special cases only through generalized *position* co-ordinates, i.e. asymptotic phase-shifts - again generalizing §4.1. Despite normal-mode energy separability, the phase space for *extended* modes *is* affected by the local mode environment: it is then natural to try to generalize the calculation of §4.1 by discretizing the system and attempting to keep track of mode sharing. We will discuss below the problems with this approach for modes whose density can be large, but first we illustrate these difficulties for SG.

The inverse scattering transform (IST) allows us to perform a canonical transformation from $\{\phi, \phi_x, \phi_t\}$ to variables effectively labeling "position", "velocity", "frequency" of component nonlinear modes. For SG, there is (i) a continuous spectrum (extended modes or "radiation") parametrized by "momentum" $p = \hbar k(-\infty < p < \infty)$; $\rho(p)$ (density of states) $(0 \leq \rho(p) < \infty)$ and $\phi(p)$ $(0 \leq \phi(p) < 2\pi)$ constitute action-angle variables as in harmonic theory with similar Poisson brackets $\{\phi(p), \rho(p')\} = \delta(p-p')$. (ii) a finite number of kink-soliton variables p_j (asymptotic "momentum") and q_j (initial "position") (see §2A). ($-\infty < p_j, q_j < \infty$) and $\{p_j, q_j\} = \delta_{j,k}$. (iii) a finite number of breather co-ordinates $p_j^B, q_j^B(-\infty < p_j^B, q_j^B < \infty)$, $\alpha_j^B(0 < \alpha_j^B < \pi/2)$, $\beta_j^B(0 < \beta_j^B < 4\pi E_K^{(0)} \omega_0^{-1})$. α_j^B is related to the internal frequency of the j-th breather ($\cos \alpha_j \approx \omega_j/\omega_0$; see (5)) and β_j is related to the phase angle of the breather oscillation. The Hamiltonian separates as [27] (c.f. §2A)

$$H = \int_{-\infty}^{\infty} dx\, \mathcal{H}(x) = \int_{-\infty}^{\infty} dp\, \rho(p)(p^2 c_0^2 + h^2 \omega_0^2)^{1/2}$$

$$+ \sum_{j=1}^{N_s} \left[p_j^2 c_0^2 + E_K^{(0)2} \right]^{1/2} + \sum_{j=1}^{N_B} \left[p_j^{B2} c_0^2 + E_j^2(\alpha_j^B) \right]^{1/2} \quad . \tag{27}$$

with N_s kink solitons (and anti-solitons) and N_B breathers. The final remarkable feature is that all mode interactions are pair-wise additive. Thus asymptotic phase shifts can be taken in pairs and the low-T additivity assumption in §4.1,2 should extend rigorously to arbitrary T for kinks and breathers. Explicit expressions for linear mode phase shifts from an isolated kink, $\delta(k;v)$, (§4.1,2) or breather, $\delta_B(k;v_B,\alpha_B)$, (below) are available [27].

These circumstances make the conceptual generalization of the low-T partition function calculation immediate. We discretize on a finite length L, assume (27) still holds and assume continuum phase-shifts. Indeed the calculation for kinks was given for an arbitrary kink velocity, so that (22) is unchanged. Following a parallel procedure for breathers we need $\Delta F_B(v_B,\alpha_B)$, the change in extended ("phonon") mode free energy density due to a single breather: $L\Delta F_B(v_B,\alpha_B) = k_B T\, P \int \frac{dk}{2\pi}\, \delta_B(k;v_B,\alpha_B) \cdot n(\beta h\omega_k)$, i.e.

$$L\Delta F_B(v_B,\alpha_B) \xrightarrow{\ \ d\ \ } -2k_B T\, n(\beta h\omega_0)$$

$$+ \frac{k_B T}{2\pi} P \int_{-\infty}^{\infty} dk\, \frac{d\delta_B}{dk}(k;v_B,\alpha_B) \cdot n(1 + k^2 d^2)^{1/2}$$

$$- 2k_B T \cdot n(\beta h\omega_0) + \frac{k_B T}{4\pi} \int_{-\infty}^{\infty} dk\, \frac{d\delta_B}{dk}(k;0,\alpha_B) \cdot n(1+k^2 d^2), \tag{28}$$

where we have used a Lorentz-boosted phase-shift (c.f. §4.1); $P\int dk(d\delta_B/dk) = -4\pi$ (corresponding to the removal of two linear modes per breather - a breather can be viewed as a kink-antikink bound state); and $d\delta_B/dk$ is even in k - $d\delta_B/dk$ is the part of $d\delta_B/dk$ analytic on the real k-axis. $d\delta_B(k,0,\alpha_B)/dk = -4d(1 - \omega_B^2/\omega_0^2)^{1/2}(1 + k^2 d^2 - \omega_B^2/\omega_0^2)^{-1}$ to be compared with the corresponding kink expression $d\delta(k,0)/dk = -2d(1 + k^2 d^2)^{-1}$. (The breather result = twice the kink result as $\omega_B \to 0$.) Evaluating (28), we define a renormalized breather energy ($\epsilon = (1-\omega_B^2/\omega_0^2)^{1/2} = \sin\alpha_B$)

$$E_B^*(\alpha_B,\beta_B) = 2\epsilon_B E_K^{(0)} - 2k_B T \cdot n[\beta h\omega_0(\epsilon...)] \tag{29}$$

to be compared with (20), especially as $\omega_B \to 0$. Using asymptotic phase-shift additivity and Hamiltonian separability, we can now extend (21) by including an extra grand canonical partition function for breathers

$G_B(T,L,\mu_B) = \sum_{N_B=0}^{\infty} \exp(\beta\mu_B N_B) Z_B(N_B)$ with $Z_B(N_B) = (N_B!)^{-1} Z_B^{N_B}$ and

$$Z_B = h^{-2}\int_{-\infty}^{\infty} dp_B \int_0^L dq_B \int_0^{\pi/2} d\theta_B \int_0^{4\pi E_K^{(0)}/\omega_0} d\beta\, \exp[-\beta E_B^*(p_B,\omega_B)] \text{ giving}$$

$$Z_B = \frac{4L}{\pi d}\left(\beta E_K^{(0)}\right)^2 \int_0^1 d\nu \int_1^{\infty} d\gamma\, \frac{\eta(\gamma+\gamma)^2\, e^{-2\beta E_K^{(0)}\nu\gamma}}{(\gamma^2-1)^{\frac{1}{2}}\,(1-\nu^2)^{\frac{1}{2}}} \quad . \tag{30}$$

(Note how the phase shift effects cancel powers of h in (21) and (30), a feature lost if we use *pure* ideal relativistic gases.) We presented this calculation to illustrate some characteristic problems (below). Note already the renormalization of E_B (eq. (29)) even as $\omega_B \to \omega_0$, the harmonic limit. This limit ($\omega_B \to \omega_0$; $\eta \to 0$) is the source of many related difficulties: (30) can be evaluated tediously in terms of modified Bessel fns., with low-T expansion

$$Z_B \xrightarrow{\beta E_K^{(0)} \gg 1} \frac{3L}{2d}\left\{1 + \frac{2}{3}\left(\beta E_K^{(0)}\right)^{-1} + O\left(\beta E_K^{(0)}\right)^{-2} + \frac{4}{3}\int_0^1 d\nu\, \frac{K_1(2\beta E_K^{(0)}\nu)}{\nu(1-\nu^2)^{\frac{1}{2}}}\right\} \tag{31}$$

The reader can check the several unhappy features in (31): for instance, the breather density $n_B(T) = Z_B/L$ (assuming $\mu_B = 0$), and the free energy density is $F = F_0 - k_BTn_K - k_BTn_B$, to be compared with the TIO result for SG[2]: $F = F_0 - k_BTn_K - (k_BT/4d)(\beta E_K^{(0)})^{-1} + O((k_BT)^3/E_K^{(0)3})$. Even more indicative is the explicit *divergence* of the remaining integral (for any finite T) in (31) *as* $\omega_B \to \omega_0$ (dominantly from $\omega_B/\omega_0 \gtrsim 1 - \frac{1}{8}(k_BT/E_K^{(0)})^2$). These problems arise from our lack of control over mode conservation and taking a consistent thermodynamic limit (below). They are quite generic to gapless *envelope* solitons: for instance, we have found the *same* difficulties in analyzing *classical* SM for the cubic Schrödinger equation or the isotropic continuum ferromagnet (2C), for which mode-sharing from asymptotic phase-shifts can also be established (see also [28]). Slightly more control may be possible for *pulse* solitons as in the Toda lattice, even though they also have a gapless energy spectrum. For instance YOSHIDA [22] has used *infinite* chain action-angle variables (for "solitons" and "ripples") on a finite chain and imposed periodicity and mode conservation by hand (restricting ripple wave-vectors). In this way he finds agreement with TIO results at *low* T. Here again, however, controlled use of phase-shift information is more appropriate (work in progress) as well as integrability structure for the *finite* discrete chain (below). For *kink* solitons (i.e. finite energy gap) we saw (§4.1) that exact agreement with TIO could be obtained at *low* T. In view of SG integrability, it might be thought that result (22) would give an exact kink description at all T. In fact comparing with the predicted [19] n_K from correlation lengths in TIO, we find that (22) is a slightly *worse* prediction than the asymptotic formula (23). This seems to argue for the importance of non-trivial mode interactions on a discrete SG chain with periodic boundary conditions. [We note in passing, however, that it is advantageous [29] to use E_K^* (eq. (20)) to construct an "ideal gas" velocity distribution - as used in phenomenological structure factor models.]

We now briefly summarize the difficulties of using available IST mathematics to construct a classical SM (see also [2]). They are all consequences of a gapless spectrum or of high T.

(i) we have implicitly assumed above that there is no special distinction of multiple occupations of the same "soliton state" (specified by positions of poles and pairs of poles in the eigenvalue plane in inverse scattering theory). In general this is untrue which will be important for high soliton densities (from pulses, envelopes or, at high T, kinks).

(ii) The possibility of arbitrarily low energy breathers and correspondingly large densities, and spatial extensions' means that consistent mode counting is more sensitive than for a low density of local kinks. The canonical action-angle variables and phase-shifts used above were strictly valid for a continuum system with decaying boundary conditions. The use of these data for a finite discrete system with periodic boundary conditions (as used for TIO) is clearly uncontrolled as is the process of taking the thermodynamic limit. (Finite gap, localized kink excitations were insensitive to these concerns.) One can try to enforce mode conservation and soliton size cut-off in approximate ways, but the most desirable route is to construct SM with IST data for a finite, discrete, integrable system with, e.g., periodic boundary conditions, and *finally* take the thermodynamic limit. This is on-going work: IST status for such problems is summarized by McLAUGHLIN. The Toda lattice is especially attractive as well as some discrete spin models related to discrete generalizations of non-linear Schrödinger.

(iii) *Classical* SM was implied in TIO by the separation $Z = Z_\phi Z_i$ (§3.1). It was implemented in our nonlinear phenomenology by the use of high-T ($k_BT \gg \hbar\omega_0$) harmonic phonon free energy expressions (e.g. (18)). There is some inconsistency therefore in our use of a purely *classical* breather spectrum, especially for low energy (extended) breathers with $E_B \lesssim \hbar\omega_0$. (This problem is intrinsic to the dual particle-oscillator character of breathers and related solitons.) In particular the *quantum* breather spectrum is *discrete*. This is often not serious for applications but in for low-energy breathers since the *lowest* energy breather is physically equivalent to the quantum harmonic oscillator, i.e. Klein-Gordon quantum. (c.f. the classical spectra (§2A).) Indeed any breather may be viewed as a multi-magnon (or phonon, etc.) bound state: breathers and solitons exhaust the quantum SG spectrum. While it is a technically challenging problem to construct a truly classical SM (for arbitrary T), this was not really achieved even for kinks (§4.1) and physical concern necessarily centers on *quantum* SM from which a high T (classical) limit can be extracted if desired. It is therefore our opinion that a major effort should now be devoted to quantum SM of "soliton" systems. Quantization schemes for nonlinear objects will be reviewed separately by MAKI: some useful progress has been made in constructing a quantum SM for ϕ-four, SG and double quadratic, etc. (§2A) using nonlinear generalizations (analogous to classical collective co-ordinate manipulations, §4) of conventional *perturbative* functional integral formalisms. An alternative approach is to concentrate on fully *integrable quantum* Hamiltonians (including SG), particularly motivated by connections with *Bethe ansatz* literature [30]: see also BONNER, EMERY, McLAUGHLIN. We do not have space to describe this philosophy here: details will be published elsewhere. The basic ingredients are [30] (i) the unification of the majority of soluble many-body models as integrable quantum Hamiltonians with explicit connections to a generalized Bethe ansatz; (ii) physical understanding of elementary "soliton" excitations from integrable *classical* Hamiltonian predecessors [12]; (iii) use of quantum SM from Bethe ansatz literature (e.g. for the spin-½ Ising-XY-Heisenberg model, with connections to both SG-like and Schrödinger-like integrable Hamiltonians).

6. Outlook

We hope that the central role of solitons in large ar[illegible] of 1-D physics will be apparent from other talks at this Meeting - e.g. AXE, BAK, BONNER, EMERY, RICE, SCHRIEFFER, STEINER, as well as contributions to the soliton session. As far as statistical properties are concerned, we suggest among important future areas: (i) exploitation of quantum integrability, the Bethe ansatz and soluble model equivalences; (ii) study of impurity effects on soliton SM (classical and quantum); (iii) study of turbulent transitions and fully-developed turbulence in driven, damped soliton systems with thermal noise (having potential lessons for both solid state and fluid turbulence theory). These are all on-going projects.

References

1. A. R. Bishop, in *Solitons and Condensed Matter Physics*, eds. A. R. Bishop, T. Schneider (Springer, Berlin, 1978).
2. J. F. Currie et al., Phys. Rev. B22 (1980); A. R. Bishop et al., Physica D1, 1(1980); A. R. Bishop et al., Adv. in Phys., in prep.
3. e.g. R. Jackiw, Rev. Mod. Phys. 49, 681(1977).
4. S. F. Edwards and A. Lenard, J. Math. Phys. 3, 773(1962).
5. A. Seeger and P. Schiller, in *Physical Acoustics*, ed. W. P. Mason (Academic, N.Y., 1966), Vol. 3.
6. J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B11, 3535(1975).
7. R. M. DeLeonardis and S. E. Trullinger, preprint (1980); and refs.
8. A. R. Bishop, unpublished (1975).
9. J. F. Currie et al., Phys. Rev. A20, 2213(1979).
10. S. E. Trullinger and R. M. DeLeonardis, preprint (1980); K. R. Subbaswamy and S. E. Trullinger, preprint (1980).
11. A. Patkós and P. Ruján, Z. Physik B33, 163(1979); P. S. Riseborough and S. E. Trullinger, preprint (1980).
12. e.g. L. A. Takhtajan, Phys. Lett. 64A, 235(1977); A. E. Borovik, Pisma JETP 28, 629(1978); E. K. Sklyanin, preprint (1980).
13. K. A. Long and A. R. Bishop, J. Phys. A12, 1325(1979).
14. A. R. Bishop, et al., J. Phys. C(Lett.) 13 (1980); and in prep.
15. V. E. Zhakarov and L. A. Takhtadzhan, Teor. i Mat. Fiz. 38, 26(1979).
16. D. J. Scalapino et al., Phys. Rev. B6, 3409(1972); and refs.
17. A. R. Bishop, preprint (1980).
18. e.g. N. Gupta and B. Sutherland, Phys. Rev. A14, 1790(1976); J. F. Curie et al., Phys Rev. A16, 796(1977).
19. A. R. Bishop, Solid State Comm. 30, 37(1979); see also A. R. Bishop and J. A. Krumhansl, Phys. Rev. B12, 2824(1975).
20. S. Goldstein, Proc. Roy. Soc. (Edinburgh) T49, 210(1929); R. M. DeLeonardis and S. E. Trullinger, Phys. Rev. B20, 2603(1979).
21. e.g. H. Büttner and F. G. Maertens, Solid State Comm. 29, 663(1979).
22. F. Yoshida, private communication (1980).
23. e.g. R. Landauer and J. A. Swanson, Phys. Rev. 121, 1668(1961); J. S. Langer, Annal. Phys. (NY) 14, 108(1967).
24. e.g. G. F. Mazenko and P. S. Sahni, Phys. Rev. B18, 6139(1978); W. Apel et al., Z. Physik B 34, 183(1979); S. Coleman, Phys. Rev. D15, 2929(1977).
25. N. Theodorakopoulos, J. Phys. A12, L211 (1979).
26. S. E. Trullinger, Phys. Rev. B22 (1980).
27. J. F. Currie, Phys. Rev. A16, 1692(1977); V. E. Korepin and L. D. Faddeev, Physics Reports C 42, 1(1978).
28. H. C. Fogedby, Physica Scripta (in press).
29. S. E. Trullinger and A. R. Bishop, preprint (1980).
30. A. R. Bishop, Z. Physik B 37, 357(1980); and refs.